

# The Rayleigh Quotient

M. K.G. Kruse<sup>a</sup>, J. M. Conroy<sup>b</sup> and H. G. Miller<sup>b</sup>

<sup>a</sup>*Physics Department, University of Arizona, Tucson, Arizona, USA*

<sup>b</sup>*Physics Department, SUNY Fredonia, Fredonia, NY, USA*

The central role of the Rayleigh quotient in many body physics is discussed. Various many body methods can be obtained from either an attempt to evaluate the Rayleigh Quotient directly or through various variational approximations. Rather than dwell on the technical details necessary to obtain the equations of the various many body methods, we concentrate on how they can be obtained from the Rayleigh Quotient, and some of the consequences of the approximations involved in their evaluation.

Many of the approximation schemes employed in quantum mechanics can be gleaned by simply considering the minimization of the Rayleigh quotient

$$\delta\left(\frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle}\right) = 0 \quad (1)$$

where  $\psi$  is the many body wave function and  $\hat{H}$  is the many body Hamiltonian operator. Clearly in order to perform the variation, the Rayleigh quotient must exist and be finite. This immediately rules out the possibility of determining scattering states from equation (1) as they are not normalizable in the usual  $\mathcal{L}^2$  sense. Furthermore, if the operator,  $\hat{H}$ , is not bounded in some manner the Rayleigh quotient does not possess a bound and the variational problem is no longer valid.

In what follows, we shall assume that the Hamiltonian operator possesses at least one bound, and for simplicity that it is bounded from below. If, for example,  $\hat{H}$  possesses only a point spectrum (*i.e.* only a bound state spectrum) it must have at least a state of lowest energy (a ground state). However, the space spanned by the many body wave functions need not necessarily be finite only denumerable. In this case, if no restriction is placed on the class of many body trial functions other than they be normalizable, equation(1) yields the many body Schroedinger eigenvalue equation

$$\hat{H}\psi = E\psi \quad (2)$$

which is valid for every many body eigenfunction,  $\psi$  whose corresponding eigenvalue (or eigenenergy) is  $E$ . The many body state with the lowest energy corresponds to the ground state.

Note, however, that most many body Hamiltonian operators support not only a bound state spectrum but also scattering states. The spectrum of bound states is therefore not complete. Although each eigenstate of such Hamiltonian operators may be expanded in a complete set of basis states, a simple unitary transformation between the eigenstates of said Hamiltonian operator and any set of complete basis states does not exist. This, of course, may lead to problems if the solution of equation(1) (exact or approximate) is expanded in an arbitrary set of basis states. Spurious solutions may occur[1–3].

Now, in general, even if the space spanned by the many body eigenfunctions is finite and denumerable, it is usually massive and a representation of the operator  $\hat{H}$  in terms of many body basis states, yields a matrix which far exceeds the storage capacity of even the largest computers. For this reason a variety of approximation methods have been developed and often are referred to as many body techniques.

A conceptually simple way to make the problem tractable is to map the Hamiltonian operator onto a small subspace in a manner first suggested by Bloch and Horowitz[4]. The effective operator obtained should have the same eigenvalues as the original Hamiltonian operator. Unfortunately the method is fraught with difficulties. The effective Hamiltonian is non-linear and no longer Hermitian and the resulting effective Schroedinger equation is no longer a simple eigenvalue equation. Problems arising from truncation of the remaining part of the many body space in the construction of this operator occur. Furthermore the solution of the effective Schroedinger equation yields only the projection of many body eigenfunctions onto the small subspace, which necessitates the construction of effective operators corresponding to any other desired observables. Improvements of the method have been made[5, 6].

A simple power series expansion of the eigenpairs of  $\hat{H}$  yields the well-known perturbation expansion, which is a standard technique in quantum mechanics, in spite of the fact that the radius of convergence of this series is often unknown. Even for the simplest of potentials in one dimension ( $V \propto \frac{1}{x^n}$  for  $n \geq 5/2$ ) perturbative techniques fail, and more complicated expansions involving re-summation techniques must be used[7].

Rewriting equation (2) as an integral equation yields via Green's method, iterative schemes for obtaining the eigenpairs. Unlike as in the case of scattering, where the energy in the Green's function is given, in the bound state

problems the eigenenergy of the desired eigenstate must be known, in order to determine the required Green's function. Simple techniques in 1D have been developed to determine both the eigenfunctions as well as the eigenenergies[8]. In the case of infinite systems in 3D, more complicated techniques, which involve summations of the embedded two particle interactions, G-matrix expansions have been used with success. These have been shown to be equivalent to coupled cluster expansions which have also been employed in finite systems.

Techniques based on the Raleigh-Ritz method such as finite basis approximations as well as the Lanczos algorithm[9] have also been employed. In this case a small number of basis states are selected and the Hamiltonian operator is diagonalized in this subspace. In calculations performed in atomic physics sum rule considerations are used as a criterium to select the space spanned by these basis states[10]. In the case of the Lanczos algorithm[11] an orthonormalized set of Krylov vectors[12] is used to construct iteratively a matrix representation of  $\hat{H}$  which is then diagonalized. However, as has been pointed out, spurious solutions may occur[2], but can be identified easily[1, 3].

Alternatively, approximations to the many body wave function may be made either before, or after the variation of the Rayleigh quotient. Restricting the class of trial wave functions before variation leads to many of the standard variational techniques developed in many body physics. For example, restricting the trial many body wave function to a single Slater determinant (an antisymmetrized product of single particle orbitals or wave functions) yields the well known Hartree Fock (HF) equations. In spite of the fact that the variation is a linear operation, the fact that it is applied in a product space of single particle orbitals, leads to a non-linear set of equations, which must be solved iteratively. Although the solution of the HF equations corresponding to the ground state is often obtained by diagonalizing the non-linear HF Hamiltonian operator, no mathematical proof of convergence exists. However, considerable numerical evidence exists that this algorithm is convergent and yields a simple approximation of the exact ground state. More complicated choices of the trial wave function lead to the multi-configurational HF equations and the introduction of quasi-particles into the ansatz for the orbitals used in the trial wave function lead to other approximation schemes, for example the HFB and the BCS approximation schemes.

An additional approximation may be made by using a finite basis expansion for the variational state. In the HF case, one obtains the Hartree-Fock-Roothaan (HFR) equations[13]. While it is clear that Hartree-Fock single particle orbitals can be expanded in an appropriately chosen finite set of basis states, an *a priori* choice of basis states need not necessarily lead to the same ground state solution of the HF and HFR equations.

In both finite basis approximations, as well as in variational methods such as HFR, the choice of the set of basis states is extremely important. In atomic physics, where finite basis approximations are employed, sum rule considerations are routinely used to select the space spanned by the basis functions[10]. In nuclear physics, the presence of low-lying collective states, strongly suggests that relatively few properly chosen basis states are required[14, 15]. This being the case, it has been suggested that one could use extended variational methods, based on the HF approximation, to generate a set of orthogonal basis states to use in a Rayleigh Ritz calculation of the exact eigenstates[16, 17].

On the other hand, one might try to simply evaluate the Rayleigh quotient exactly using path integrals. The path integral approach to many body systems typically involves the selection of an overcomplete set of states[18–22]. For example, coherent states are a particularly useful choice, since they are eigenstates of the annihilation operator, thus simplifying the evaluation of matrix elements. Coherent states also yield a resolution of unity that makes constructing many body functional integrals simpler. Recent progress has been made regarding the efficiency of numerical evaluations of these path integrals (e.g. [23, 24]). For a particular overcomplete set of states, classical equations of motion can be obtained using the standard saddle-point approximation. Different choices in the overcomplete set produce different classical approximations. For example, by choosing the set of all Slater determinants, one obtains the Time-dependent Hartree-Fock Equations. As pointed out in [20], the choice of a particular overcomplete set is equivalent to a particular choice of trial wavefunctions in the variational principle. Moreover, the functional integral approach provides a way of calculating corrections to the classical approximation.

Alternatively one might use Monte Carlo techniques to evaluate the multi dimensional integrals in the Rayleigh quotient. In the earlier Shell Model Monte Carlo (SMMC) method[25] statistical mechanical techniques were used to reduce the imaginary many body evolution operator to a coherent superposition of fluctuating one body fields. The resulting path integral is evaluated stochastically. Difficulties arise when the weights used in the evaluation of observables are not positive. This sign problem occurs for many body Hamiltonians used in nuclear physics calculations. In the Quantum Monte Carlo Diagonalization[26], stochastic sampling of the many body states is used to select only those states, which are important to the eigenstate to be obtained. The ground state is obtained by performing a diagonalization of the Hamiltonian operator in this basis.

Full configuration interaction methods (full CI), in which a single reference state is used, from which all  $n$ -tuple excitations are generated, are always one of the best possible many-body calculation that one can do, but unfortunately is limited by current computational abilities. However, there are techniques which approximate full CI calculations, one of which is the method of coupled cluster [27]. Coupled cluster methods also have the advantage that the calculated energies scale properly with system size, (*i.e.*, linearly in particle number). This property is known as size-extensivity. In most many body calculations, the idea of size-extensivity, as well as the closely related property

of size consistency is often overlooked. These two ideas are related, and so, to avoid confusion, we will briefly describe them. Size-consistency is most easily understood from the viewpoint of a chemical reaction. The dissociation of a single system, “AB”, into two parts, system A and B, which eventually are infinitely separated from each other, should give the same total energy as the original system “AB”. In other words,  $E_{AB} = E_A + E_B$ . To mathematically define size consistency is very difficult, and arguments as to whether quantum systems are ever truly separated arise [28]. Size extensivity on the other hand, states that the energy of a system, such as an electron gas, should scale linearly with the number of particles present. Such an idea is much easier to formulate mathematically. In terms of approximation methods used in many-body techniques, size extensivity is discussed much more frequently, and is often the most desired property, whereas size consistency is usually an afterthought. The most logical step is to limit CI calculation to single and double excitations, often abbreviated as CI-SD. In this case, the CI-SD wavefunctions are generated as follows,  $\Psi_{\text{CISD}} = (1 + \hat{C}_1 + \hat{C}_2)\Phi_0$ , in which  $\Phi_0$  is the single Slater determinant used as a reference function, and the  $\hat{C}_i$  are the operators that generate the single and double excitation on top of the reference function.

Unfortunately this truncation scheme lacks size extensivity. This effect was first noticed by Brueckner in studies of the electron gas [29], where the number of particles  $N$  goes to infinity. The energy should be linear in  $N$ , but terms arising from the Raleigh-Schroedinger perturbation theory (RSPT) expansion contained terms that were proportional to  $N^2$  and  $N^3$ . Brueckner showed that these unphysical terms are canceled up to fourth order. Goldstone demonstrated that these unphysical terms cancel to all orders [30], since the perturbation terms can be decomposed into linked and unlinked diagrams. The unlinked diagrams are the terms that destroy size extensivity, but provided one does RSPT to infinite order, are always canceled out. This is the linked diagram theorem. CI calculations are related to RSPT expansions, in order to extract the CI eigenvalues. In the case of CI-SD, the calculation retains these unlinked diagrams that are proportional to  $N^2$  etc, and are thus not canceled out. The cancellation occurs if one were to add more excitations to the CI calculation, such as CI with singles, doubles, triples and quadruples included. Unfortunately, unlinked diagrams will still remain, since they are canceled by an ever higher order of excitation. The complete cancellation of unlinked diagrams only occurs once all excitations are included, but this brings us back to the computational problems of full CI.

Size extensivity can be restored in the RSPT expansion. The extensivity is restored if one considers all configurations to a given order. This leads to many-body perturbation theory (MBPT), which is a fully-linked diagrammatic expansion, order by order, and thus size extensive, up to that given order [27, 31]. Unfortunately, each subsequent order is more difficult to calculate than the previous one, rendering the method useful, but not efficient. Coupled cluster (CC) offers a slightly different approach to the problem, by providing an infinite order resummation of MBPT in selected clusters, such as single and double excitations. CC is by construction size extensive. Although CI and CC both have the same inherent ideas, *i.e.* generate single and double excitations on top of a reference state, the difference to CI comes from the exponential ansatz made in CC. The coupled-cluster wavefunction is generated by  $\Psi_{\text{CC}} = \exp(T)\Psi_0$ , where  $T = T_1 + T_2 + \dots + T_n$ , where  $T_p$  is a connected cluster operator that generates the  $p$ -fold excitation. It is this exponential form which ensures the size extensivity of the method. In the case of single and double excitations, one speaks of CCSD calculations. CCSD actually builds in more correlations than CISD would, since the exponential expansion generates terms such as  $T^2/2$  and  $T_1T_2$ . Although CC has some advantages over CI, such as being size extensive and more efficient, it is not as versatile as truncated CI. In the case of nuclear structure, CC is often used to calculate the ground state energies of doubly-magic nuclei, such as  $^{40}\text{Ca}$  [32]. Recently, CC in nuclear structure has been extended to  $A \pm 2$  nuclei, in which  $A$  represents a doubly magic nucleus [33]. For other nuclei, the techniques of CI are commonly used.

In the preceding few paragraphs, we have discussed the role of size extensivity in many-body calculations. Although CC is size extensive, it does suffer from another difficulty, related to the truncation of the basis and the introduction of contamination of the many-body wavefunction with center of mass motion. Both CI and CC have their basis truncated at the single particle level. On the other hand, the basis used in the No-Core Shell Model (NCSM) [34], a method for calculating observables of light nuclei from an *ab-initio* viewpoint, has its basis truncated at the level of energy quanta. In nuclear structure, CI, CC and the NCSM all use as single particle states the harmonic oscillator functions,  $\psi_{nljm}(r)$ . The single particle states are antisymmetrized to form Slater determinants, forming the many-body basis, in which the diagonalization is done. Returning to the two different truncation schemes, in CI-SD and CCSD, two particles could be placed in single-particle states that correspond to the highest single-particle energy possible. For example, if we truncate our basis at the  $2\hbar\omega$  level on top of a reference state build up of only 0s components, we could place our two particles in any of the *sd*-shell single particle states. On the other hand, in the NCSM, the truncation is defined by sharing  $2\hbar\omega$  units of energy between the  $A$  nucleons present. In this case, we could place our two particles in the *p*-shell, or place one particle in the *sd*-shell, and the other particle in the *s*-shell. This subtle difference has implications for the separation of center of mass and intrinsic states.

The nuclear Hamiltonians that are solved in nuclear structure are initially translationally invariant. However, due to our methods of solving the Hamiltonian in a single particle basis (and not relative coordinates), we introduce states that correspond to the center of mass motion of the nucleus. These states can be separated out by the Lawson projection,

if the many-body wavefunction factorizes into an intrinsic and center of mass term,  $\Psi(\vec{x}, \vec{X}_{cm}) = \psi(\vec{x}) \otimes \psi(\vec{X}_{CM})$ , in which  $x$  represents the  $3(A - 1)$  position coordinates and  $\vec{X}_{CM}$  represents the center of mass coordinate. This factorization is guaranteed when the basis is truncated as it is in the NCSM, but not when the truncation is performed at the single particle level. The single particle harmonic oscillator functions are related to relative and center of mass coordinates through the Talmi-Brody-Moshinsky brackets [35], which is an orthogonal transformation between the two coordinate systems. However, the transformation involves the sum over expansion coefficients, in which the sum is restricted to the maximal energy quanta two nucleons may share among each other. In the case of CC, the question of center of mass contamination has been recently investigated, and a factorization has been found, although it is not clearly understood [36].

When we relate this to the Raleigh quotient, we find that although approximate methods can be used, even with proper extensive scaling, their mere formulation on the number of excitations built into the technique (such as singles and doubles etc), is not sufficient to converge to the true eigenvalues of the Hamiltonian; one needs to consider the effects of the actual basis too, since substantial error can occur, such as those caused by center of mass contamination.

In this brief note we have attempted to point out the central role of the Rayleigh Quotient in many body physics. Rather than dwelling on the technical details necessary to obtain the relevant equations of the various many body methods, we have concentrated on how they can be obtained from the Rayleigh Quotient, and some of the consequences of the approximations involved in their evaluation.

- 
- [1] R. C. Andrew and H. G. Miller, Phys. Lett. A **318**, 487 (2003).
  - [2] R. C. Andrew and H. G. Miller, J. Phys. A **41**, 158001 (2008).
  - [3] R. C. Andrew, H. G. Miller, and G. D. Yen, Chem. Phys. Lett. **475**, 298 (2009).
  - [4] C. Bloch and J. Horowitz, Nucl. Phys. **8**, 91 (1958).
  - [5] K. Suzuki and S. Y. Lee, Prog. Theor. Phys. **64**, 2091 (1980).
  - [6] K. Suzuki, Prog. Theor. Phys. **68**, 246 (1982).
  - [7] H. G. Miller, J. Math. Phys. **35**, 2229 (1994).
  - [8] D. Waxman, J. Phys. A **31**, 1329 (1998).
  - [9] C. Lanczos, J. Res. Nat. Bur. Stand. **45**, 255 (1950).
  - [10] S. P. Goldman and G. W. F. Drake, Phys. Rev. **A25**, 2877 (1982).
  - [11] W. R. Davis, ed., *Cornelius Lanczos Collected Published Papers with Commentaries*, vol. V (North Carolina State University, Raleigh, NC, 1998).
  - [12] B. N. Parlett, *The Symmetric Eigenvalue Problem* (Prentice Hall, Englewood Cliffs, N. J., 1980).
  - [13] C. C. J. Roothaan, Rev. Mod. Phys. **23**, 69 (1951).
  - [14] M. H. Macfarlane and A. P. Shukla, Phys. Lett. B **35**, 11 (1971).
  - [15] T. Dytrych, K. D. Sviratcheva, C. Bahri, J. P. Draayer, and J. P. Vary, Phys.Rev.Lett. **98**, 162503 (2007).
  - [16] H. G. Miller, R. M. Dreizler, and G. D. Dang, Phys. Lett. B **77**, 119 (1978).
  - [17] H. G. Miller and R. M. Dreizler, Nuclear Physics A **316**, 32 (1979).
  - [18] J. Klauder, Ann. Phys. (N.Y.) **11**, 123 (1960).
  - [19] H. Kuratsuji and T. Suzuki, Phys. Lett. **92B**, 19 (1980).
  - [20] J. Blaizot and H. Orland, Phys. Rev. C **24**, 1740 (1981).
  - [21] J. Blaizot and H. Orland, J. Phys. Lett. **41**, 53 (1980).
  - [22] G. Papadopoulos and J. Devrese, eds., *Path Integrals and their Applications in Quantum, Statistical and Solid State Physics* (Plenum, New York, 1977).
  - [23] A. Balaz, I. Vidanovic, A. Bogojevic, A. Belic, and A. Pelster, J.Stat.Mech. **2011**, 03005 (2011), 1011.5185.
  - [24] A. Bogojevic, I. Vidanovic, A. Balaz, and A. Belic, Phys.Lett. **A372**, 3341 (2008), 0804.2762.
  - [25] S. E. Koonin, D. J. Dean, and K. Langanke, Annual Review of Nuclear and Particle Science **47**, 463 (1997).
  - [26] M. Oysuka, T. Mizusaki, and M. Honma, J. Phys. G **25**, 699 (1999).
  - [27] R. Bartlett and M. Musial, Rev. Mod. Phys. **79**, 291 (2007).
  - [28] W. Duch and D. Dierksen, J. Chem. Phys. **101**, 3018 (1994).
  - [29] K. A. Brueckner, Phys. Rev. **97**, 1353 (1955).
  - [30] J. Goldstone, Proc. Roy. Soc. (Lond.) A **239**, 267 (1957).
  - [31] R. J. Bartlett and G. D. Purvis, Int. J. Quant. Chem. **XIV**, 561 (1978).
  - [32] D. J. Dean, M. Hjorth-Jensen, T. Papenbrock, G. Hagen, and A. Schwenk, Phys. Rev. C **76**, 044305 (2007).
  - [33] M. Hjorth-Jensen, G. Hagen, G. R. Jansen, and T. Papenbrock, Phys. Rev. C **83**, 054306 (2011).
  - [34] S. Quaglioni, I. Stetcu, P. Navrátil, and B. Barrett, J. Phys. G: Nucl. Part. Phys. **36**, 083101 (2009).
  - [35] T. Brody and M. Moshinsky, *Table of Transformation Brackets* (Monografias del Instituto de fisica, Universidad Nacional Autonoma de Mexico, 1960).
  - [36] T. Papenbrock, G. Hagen, and D. J. Dean, Phys.Rev.Lett. **103**, 062503 (2009).